

Physical Principles in Biology  
Biology 3550  
Fall 2018

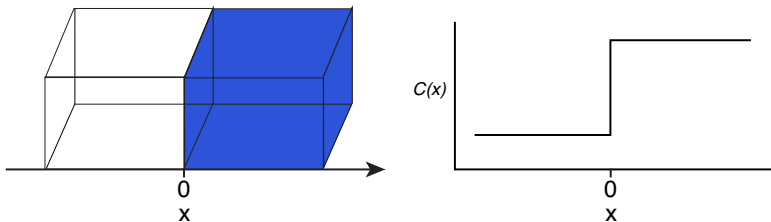
## Lecture 19:

# Thermal Energy and Molecular Motion

Monday, 15 October 2018

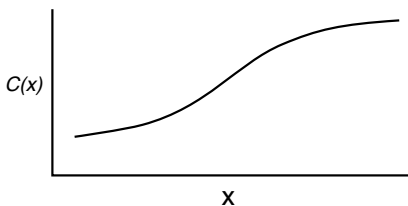
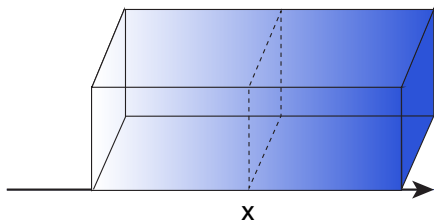
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# An Idealized Macroscopic Diffusion Experiment



- How will plot of  $C(x)$  versus  $x$  change with time?

# Fick's First and Second Laws of Diffusion



- First law:

$$J = -D \frac{dC}{dx}$$

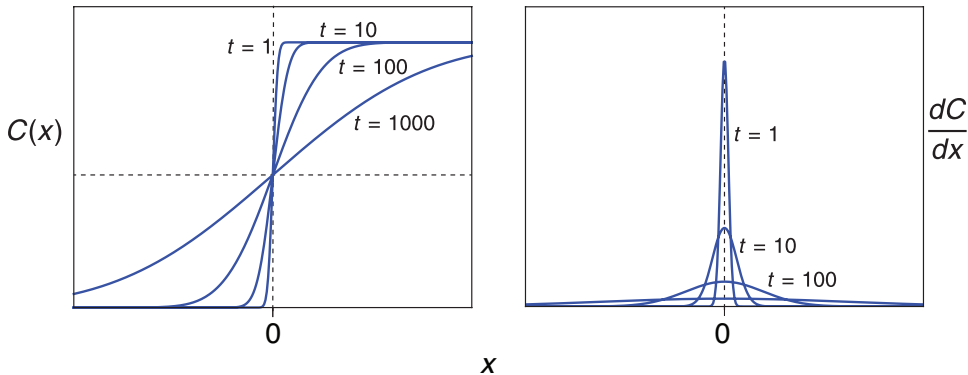
- Flux,  $J$ , at position  $x$  is proportional to the concentration gradient at that position.

- Second law:

$$\frac{dC}{dt} = D \frac{d^2 C}{dx^2}$$

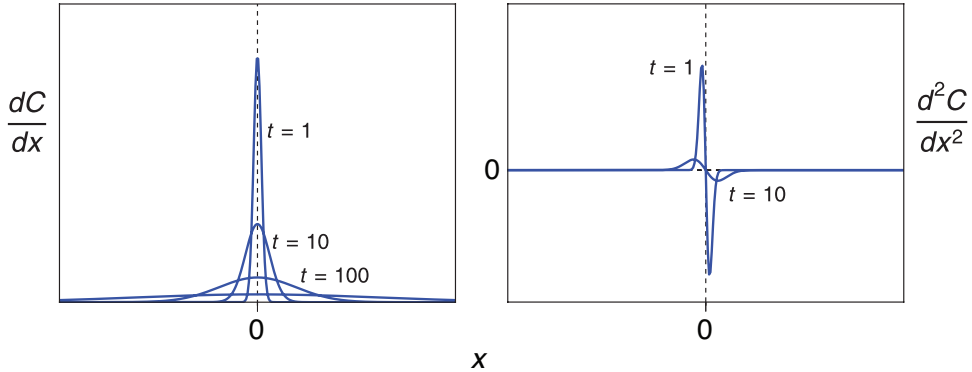
- Rate of change in concentration at position  $x$  is proportional to the derivative of the concentration gradient.

# Diffusion from a Sharp Boundary



- The derivative,  $dC/dx$  is a Gaussian function because the function  $C(x)$  is the integral of a Gaussian function!

# Diffusion from a Sharp Boundary



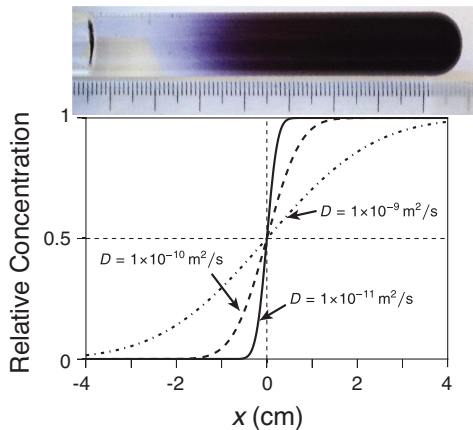
# Estimating $D$ from Diffusion from a Sharp Boundary

$$C(x, t) = \int_0^{\infty} \frac{1}{\sqrt{4\pi Dt}} e^{-(x-a)^2/(4Dt)} da$$

$$t = 48 \text{ hr} = 1.7 \times 10^5 \text{ s}$$

$$D \approx 2 \times 10^{-10} \text{ m}^2/\text{s}$$

$$D = \frac{\delta_x^2}{2\tau}$$



- What are the average length ( $\delta_x$ ) and duration ( $\tau$ ) of the random walk steps?

Warning!



Direction Change

Molecular Motion and Kinetic Energy

# Molecular Motion and Kinetic Energy

- What is energy?

Capacity to do work.

- What is work?

Mechanical work: The application of force over distance:

$$w = \int_a^b F dx$$

- The units of work and energy.

- Force: Units defined by Newton's second law:  $F = \text{mass} \times \text{acceleration}$

SI unit of mass: Kg

Acceleration: change in velocity (m/s) with time. SI units:

$$(\text{m/s})/\text{s} = \text{m/s}^2$$

SI units of Force:  $\text{Kg} \cdot \text{m/s}^2$

$$1 \text{ N} = 1 \text{ Kg} \cdot \text{m/s}^2$$

- Work or energy:  $\text{Kg} \cdot \text{m}^2/\text{s}^2$

$$1 \text{ J} = 1 \text{ N} \cdot \text{m} = 1 \text{ Kg} \cdot \text{m}^2/\text{s}^2$$



# Kinetic Energy

- A object of mass,  $m$ , moving with velocity,  $v$ , in the  $x$ -direction has kinetic energy in that direction of:

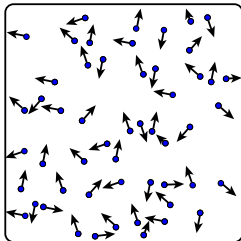
$$E_{k,x} = mv^2/2$$

Check the units:  $\text{Kg} \times (\text{m/s})^2 = \text{Kg} \cdot \text{m}^2/\text{s}^2 = \text{Nm} = \text{J}$ .     It's OK!

- What does this mean?
  - The energy required to accelerate the mass,  $m$ , from rest to velocity,  $v$ .
  - Also the energy released during the deceleration of the mass from velocity,  $v$ , to rest.
  - Kinetic energy does not depend on the rate of acceleration, only the final velocity.
  - But, amount of wasted energy likely does depend on rate of acceleration!
- $E_{k,x}$  is proportional to  $v^2$ . What are the implications?

# Kinetic Energy of Molecules

- Temperature is the measure of kinetic energy of molecules.
- How do we measure temperature?
- Pressure of a gas is due to the collision of molecules against container walls.



$$PV = nRT$$

$P$  = pressure,  $V$  = volume,  $n$  = number of moles,  $T$  = temperature,  
 $R$  = gas constant.

# Clicker Question #1

$$R = \frac{PV}{nT}$$

What are the units of the gas constant?

- A) pascal · L · K<sup>-1</sup> mol<sup>-1</sup>
- B) Kg · m<sup>2</sup> s<sup>-2</sup> K<sup>-1</sup> mol<sup>-1</sup>
- C) m<sup>3</sup> bar · K<sup>-1</sup> mol<sup>-1</sup>
- D) JK<sup>-1</sup> mol<sup>-1</sup>
- E) L · atm · K<sup>-1</sup> mol<sup>-1</sup>
- F) N · m · K<sup>-1</sup> mol<sup>-1</sup>

All of the above!

# Units of the Gas Constant

- From the ideal gas law:  $R = \frac{PV}{nT}$

- In SI basic units:

Pressure, force per unit area:  $\text{Kg} \cdot \text{m} \cdot \text{s}^{-2} \div \text{m}^2 = \text{Kg} \cdot \text{m}^{-1}\text{s}^{-2} = \text{Pa}$

Volume:  $\text{m}^3$

Gas constant:  $\text{Kg} \cdot \text{m}^2\text{s}^{-2}\text{K}^{-1}\text{mol}^{-1}$

- Joule (unit of energy) =  $\text{Nm} = \text{Kg} \cdot \text{m}^2\text{s}^{-2}$

- The gas constant expressed in energy units:

$$R \approx 8.314 \text{ JK}^{-1}\text{mol}^{-1} \approx 1.987 \text{ cal/K}^{-1}\text{mol}^{-1}$$

- $RT$  is proportional to the kinetic energy of one mole of molecules at a temperature  $T$ .

# Kinetic Energy of Molecules

- The Boltzmann constant,  $k$ , the “gas constant per molecule”:

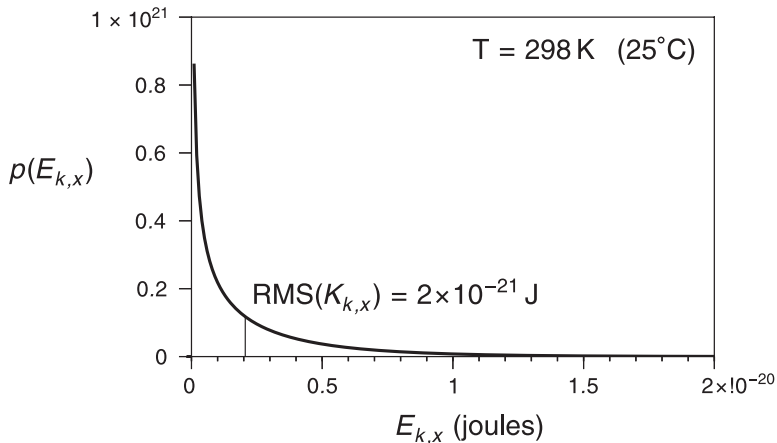
$$\begin{aligned}k &= R/N_A = 8.314 \text{ JK}^{-1}\text{mol}^{-1} \div 6.02 \times 10^{23} \text{ molecule/mol} \\ &= 1.38 \times 10^{-23} \text{ JK}^{-1}\end{aligned}$$

- Molecules at a given temperature do not have unique velocities or kinetic energies.
- Molecules have a broad distribution of energies, with RMS average kinetic energy in each direction ( $x$ ,  $y$  or  $z$ ):

$$\text{RMS}(E_{k,x}) = kT/2$$

- Translational kinetic energy does *not* depend on mass or structure.
- In context of molecular motion, “ $E_{k,x}$ ” will imply RMS value.

# Distribution of Molecular Kinetic Energies



$$p(E_{k,x}) = \frac{1}{\sqrt{\pi E k T}} e^{-E/(kT)}$$

## Clicker Question #2

How fast does a small molecule move at room temperature  
(between collisions)?

A)  $10^{-6}$  m/s

B)  $10^{-4}$  m/s

C)  $10^{-2}$  m/s

D) 1 m/s

E)  $10^2$  m/s

F)  $10^4$  m/s

All answers count for now.

# Velocities of Molecules

- Kinetic energy of a molecule, in  $x$ -direction:  $\text{RMS}(E_{k,x}) = kT/2$
- Kinetic energy of any object:  $E_{k,x} = mv_x^2/2$
- Solving for  $v$ :

$$mv_x^2/2 = kT/2$$

$$v_x^2 = kT/m$$

$$v_x = \sqrt{kT/m}$$

(also an RMS value)

- Velocity increases with  $\sqrt{T}$  and decreases with  $\sqrt{m}$ .



# Velocity of an N<sub>2</sub> Molecule at Room Temperature

- Mass

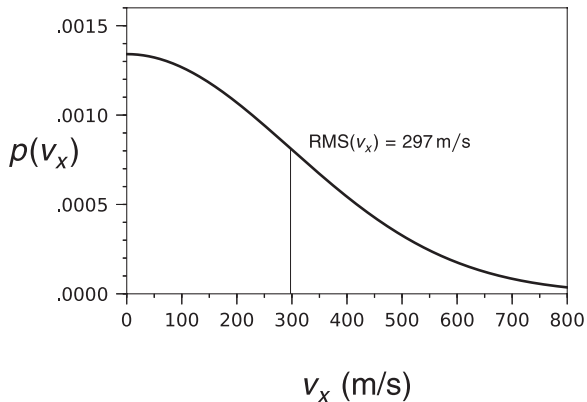
$$\begin{aligned}m &= 28 \text{ g/mol} \div 6.02 \times 10^{23} \text{ molecules/mol} \\ &= 4.65 \times 10^{-23} \text{ g} = 4.65 \times 10^{-26} \text{ Kg}\end{aligned}$$

- Temperature = 25°C = 298 K

- Velocity:

$$\begin{aligned}\text{RMS}(v_x) &= \sqrt{kT/m} \\ &= \sqrt{1.38 \times 10^{-23} \text{ Kg} \cdot \text{m}^2\text{s}^{-2}\text{K}^{-1} \times 298 \text{ K} / 4.65 \times 10^{-26} \text{ Kg}} \\ &\approx 300 \text{ m/s} \quad (1,000 \text{ km/hr})\end{aligned}$$

# Distribution of $N_2$ Velocities in a Gas at 298 K



- The Maxwell-Boltzmann distribution

$$p(v_x) = \sqrt{\frac{m}{2\pi kT}} e^{-mv_x^2/(2kT)}$$

(assumes ideal gas behavior)